1,2,3-Trichloropropene

96-19-5 | DTXSID3047766

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.49 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.15e-01

Confidence level: 4.72e-01

Nearest Neighbors from the Training Set

Image not found
1,2,3-Trichloropropane
Measured: 4.40
Predicted: 7.68

Image not found
Ethyl isovalerate
Measured: 28.4
Predicted: 6.89

Image not found
Butyl glycidyl ether
Measured: 1.88
Predicted: 2.73

Image not found
4-Methylpyridine
Measured: 12.0
Predicted: 5.43

Image not found
Decamethylcyclopentasiloxane
Measured: 5.80e-01
Predicted: 1.65e-01